Package ‘pesticides’

February 20, 2015

Type Package

Title Analysis of single serving and composite pesticide residue measurements

Version 0.1

Date 2010-11-17

Author David M Diez

Maintainer David M Diez <david.m.diez@gmail.com>

Description Single item and composite pesticide residue measurements of fifteen commodity-pesticide combinations plus analytical tools.

License GPL-3

LazyLoad yes

Repository CRAN

Date/Publication 2012-10-29 08:59:26

NeedsCompilation no

R topics documented:

pesticides-package ......................................................... 2
apple ................................................................. 3
appleAll ........................................................... 4
cdfDist ............................................................. 5
cor2icc ............................................................. 7
peach ................................................................. 8
pear ................................................................. 9
pepper ............................................................... 10

Index 12
Description

Single item and composite pesticide residue measurements of fifteen commodity-pesticide combinations plus analytical tools.

Details

```
Package: pesticides
Type: Package
Version: 0.1
Date: 2010-11-17
License: GPL-3
LazyLoad: yes
```

Author(s)

David M Diez
Maintainer: David M Diez <david.m.diez@gmail.com>

References

United States Department of Agriculture Pesticide Data Program (www.ams.usda.gov/science/pdp/).
United States Environmental Protection Agency (http://www.epa.gov/).
National Food Administration of Sweden (http://www.slv.se/en-gb/) (http://www.slv.se/upload/dokument/rapporter/kemiska/

See Also

apple, peach, pear, pepper, cor2icc, cdfDist

Examples

```r
#===== cor2icc =====#
data(apple)
pest <- unique(apple$pesticide)
icc <- rep(-1, length(pest))
for(i in 1:length(pest)){
  these <- apple$pesticide == pest[i]
  r <- cor(apple$comp[these], apple$ss[these])
  icc[i] <- cor2icc(r, 10,"within")
```
} names(icc) <- pest icc

#======> cdfDist ======#
par(mfrow=1:2)

F1 <- seq(0.001, 0.999, 0.001)[-sample(999, 300)]
x1 <- exp(quantile(rnorm(10000, 0.5, sd=0.5), F1))
F2 <- seq(0.001, 0.999, 0.001)[-sample(999, 300)]
x2 <- qchisq(F2, mean(x1))
hold <- cdfDist(x1, F1, x2, F2)
plot(hold)
summary(hold)

F1 <- seq(0.001, 0.999, 0.001)[-sample(999, 300)]
x1 <- exp(quantile(rnorm(10000, 0.5, sd=0.5), F1))
F2 <- seq(0.001, 0.999, 0.001)[-sample(999, 300)]
x2 <- qchisq(F2, mean(x1)+1)
hold <- cdfDist(x1, F1, x2, F2)
plot(hold)
summary(hold)

apple

Pesticide residue measurements for apples

Description

An abbreviated data set of appleAll data set. This data was collected by the USDA Pesticide Data Program and used to estimate the ICC for pesticides on apples.

Usage

data(apple)

Format

A data frame with 1134 observations on the following 6 variables.

pesticide  The pesticide measured.
comp  Measured composite residue.
ss  Measured single item residue.
lod  Minimum level of detection.
items  Number of items per composite.
sampID  Sample ID.
appleAll

**Source**

United States Department of Agriculture Pesticide Data Program.

**Examples**

data(apple)
these <- apple$pesticide == apple$pesticide[1]
r <- cor(apple$comp[these], apple$ss[these])
cor2icc(r, 10,"within")

---

appleAll  
*Full apple data set*

**Description**

Original USDA PDP data file for the apple data set. The apple data set is a derivative of this data set.

**Usage**

data(appleAll)

**Format**

A data frame with 1137 observations on the following 15 variables.

pesticide  The pesticide measured.
sampleID  Sample ID.
lod  Minimum level of detection.
comp  Measured composite residue.
singleWhole  Single apple measurement.
ss1  Single item measurement 1.
ss2  Single item measurement 2.
ss3  Single item measurement 3.
ss4  Single item measurement 4.
ss5  Single item measurement 5.
ss6  Single item measurement 6.
ss7  Single item measurement 7.
ss8  Single item measurement 8.
ss9  Single item measurement 9.
ss10  Single item measurement 10.
Source

United States Department of Agriculture Pesticide Data Program.

Examples

data(appleAll)

cdfDist

Distance measure for cumulative distribution functions

Description

This distance measure is useful in assessing the dissimilarity in two cumulative distribution functions, if differences in the right tail are of particular interest.

Usage

cdfDist(x1, F1, x2, F2)

Arguments

x1 | A vector of numerical values.
F1 | A vector of numerical values, where the i-th element of F1 is the CDF at value x1[i].
x2 | A vector of numerical values.
F2 | A vector of numerical values, where the i-th element of F2 is the CDF at value x2[i].

Details

This function first computes a pointwise distance at each value x as

\[ D(x) = \frac{(F1(x) - F2(x))^2}{1 - \min(F1(x), F2(x))} \]

The measure is equal to the integral of this distance over the intersection of the provided quantiles of the two CDFs, a region \((m1, m2)\). Finally, the measure is standardized by the distance of this range:

\[ \mu(F1, F2) = \frac{\int_{m1}^{m2} D(x)dx}{m2 - m1} \]

This measure was designed to penalize heavily if the right tails of the distributions were very dissimilar. A poor match in the lower tail results in only a slight increase of the measure.

The functions print, plot, and summary may be applied to the output of cdfDist.
Value

The output is a list of class "cdfDist":

- **x**: The values at which the pointwise distance was computed and then integrated over.
- **F1**: The first CDF for each value of x.
- **F2**: The second CDF for each value of x.
- **meas**: A vector representing the integral of the pointwise distance from x[1] up to each value of x. Plotting this measure with x makes it easy to see where the distance grew the fastest between the CDFs.
- **cdfDist**: The distance between the CDFs.

Author(s)

David M Diez

See Also

cor2icc, apple, peach, pear, pepper

Examples

```r
par(mfrow=c(2,2))

# Example 1
F1 <- seq(0.001, 0.999, 0.001)[-sample(999, 300)]
x1 <- quantile(rt(10000, 15), F1)
F2 <- seq(0.001, 0.999, 0.001)[-sample(999, 300)]
x2 <- qnorm(F2)
hold <- cdfdist(x1, F1, x2, F2)
plot(hold)
summary(hold)

# Example 2
F1 <- seq(0.001, 0.999, 0.001)[-sample(999, 300)]
x1 <- exp(quantile(rnorm(10000, 1, sd=1), F1))
F2 <- seq(0.001, 0.999, 0.001)[-sample(999, 300)]
x2 <- qchisq(F2, mean(x1))
hold <- cdfdist(x1, F1, x2, F2)
plot(hold)
summary(hold)

# Example 3
F1 <- seq(0.001, 0.999, 0.001)[-sample(999, 300)]
x1 <- exp(quantile(rnorm(10000, 0.5, sd=0.5), F1))
F2 <- seq(0.001, 0.999, 0.001)[-sample(999, 300)]
x2 <- qchisq(F2, mean(x1))
hold <- cdfdist(x1, F1, x2, F2)
plot(hold)
```
cor2icc

summary(hold)

#===== Example 4 =====#
F1 <- seq(0.001, 0.999, 0.001)[-sample(999, 300)]
x1 <- exp(quantile(rnorm(10000, 0.5, sd=0.5), F1))
F2 <- seq(0.001, 0.999, 0.001)[-sample(999, 300)]
x2 <- qchisq(F2, mean(x1)+1)
hold <- cdfDist(x1, F1, x2, F2)
plot(hold)
summary(hold)

---

cor2icc

**Compute the ICC based on linear correlation**

**Description**

Use the linear correlation to compute the ICC, where the linear correlation is estimated from regressing measurements on items within a group against the group value. The function may also be used to estimate the ICC when the individual is only associated with the group and does not contribute to the group average.

**Usage**

cor2icc(x, n, type = c("within", "not"))

**Arguments**

- **x**: A numerical value representing a linear correlation. If `x` is a matrix or data.frame, it is assumed that the first column represents either the single item measurements or the group measurements and that the opposite measurements be represented in the second column. Under this second scenario, the correlation is computed directly from the data.
- **n**: The number of single items within each group.
- **type**: If "within", then the measurements from each single item was included in the group measurement. If "not", then each single observation is associated with the group but not included in the group measurement.

**Value**

A numerical value representing the ICC.

**Author(s)**

David M Diez

**See Also**

cdfDist, apple, peach, pear, pepper
Examples

```r
#===== Example 1: apple data =====#
data(apple)
pest <- unique(apple$pesticide)
icc <- rep(-1, length(pest))
for(i in 1:length(pest)){
  these <- apple$pesticide == pest[i]
  r <- cor(apple$comp[these], apple$ss[these])
  icc[i] <- cor2icc(r, 10, "within")
}
names(icc) <- pest
icc
```

```r
#===== Example 2: peach data =====#
data(peach)
pest <- unique(peach$pesticide)
icc1 <- rep(-1, length(pest))
icc2 <- rep(-1, length(pest))
for(i in 1:length(pest)){
  these <- peach$pesticide == pest[i]
  r <- cor(peach$comp[these], peach$ss[these])
  n <- mean(peach$items[these])
  icc1[i] <- cor2icc(r, n, "not")
  icc2[i] <- cor2icc(r, n, "within")
}
names(icc1) <- pest
names(icc2) <- pest
icc1 # correct
icc2 # incorrect based on data collection procedure
```

---

**peach**

*Pesticide residue measurements for peaches*

**Description**

Pesticide residues for peaches from the USDA Pesticide Data Program.

**Usage**

```r
data(peach)
```

**Format**

A data frame with 4272 observations on the following 13 variables.

- **pesticide** The pesticide measured.
- **comp** Measured composite residue.
- **ss** Measured single item residue.
Pesticide residue measurements for pears

Description

Pesticide residues for pears from the USDA Pesticide Data Program.

Usage

data(pear)
Format

A data frame with 1962 observations on the following 13 variables.

pesticide The pesticide measured.
comp Measured composite residue.
ss Measured single item residue.
lod Minimum level of detection.
items Number of items per composite.
state State collected.
origin Origin of the produce.
year Year.
month Month.
day Day.
site Site.
lab Lab that completed measurements.
variety Peach variety.

Details

The number of items per composite was unavailable for this data set and was inputed as 10.

Source

United States Department of Agriculture Pesticide Data Program.

Examples

data(pear)
these <- pear$pesticide == pear$pesticide[1]
r <- cor(pear$comp[these], pear$ss[these])
cor2icc(r, 10, "not")

pepper Pesticide residue data for sweet peppers

Description

Pesticide residues for sweet peppers from the National Food Administration of Sweden.

Usage

data(pepper)
Format

A data frame with 166 observations on the following 6 variables.

- gp  Group or composite number.
- color  The color of the pepper.
- comp  Corresponding composite residue measurement.
- ss  Single item residue measurement.
- lod  Minimum level of detection.
- items  Number of items in the corresponding composite.

Details

Residues were measured for all individual peppers in this data set. This data is especially unique – and ideal – in that all single items within the composites were measured.

Source


Examples

data(pepper)
r  <- cor(pepper$comp, pepper$ss)
g  <- lm(comp ~ ss, pepper)
n  <- mean(pepper$items)
cor2icc(r, n, "within")
plot(pepper$ss, pepper$comp)
abline(g)
Index

*Topic **CDF distance**
cdfDist, 5
*Topic **CDF**
cdfDist, 5
*Topic **ICC**
cor2icc, 7
*Topic **Intracomposite correlation**
cor2icc, 7
*Topic **USDA**
apple, 3
appleAll, 4
peach, 8
pear, 9
*Topic **apple**
apple, 3
appleAll, 4
*Topic **commodity**
apple, 3
appleAll, 4
peach, 8
pear, 9
pepper, 10
pesticides-package, 2
*Topic **cumulative distribution function**
cdfDist, 5
*Topic **datasets**
apple, 3
appleAll, 4
peach, 8
pear, 9
pepper, 10
*Topic **decomposing**
cor2icc, 7
*Topic **distance measure**
cdfDist, 5
*Topic **exposure**
pesticides-package, 2
*Topic **package**
pesticides-package, 2
*Topic **peach**
peach, 8
*Topic **pear**
pear, 9
*Topic **pepper**
pepper, 10
*Topic **pesticides**
pesticides-package, 2
*Topic **pesticide**
apple, 3
appleAll, 4
cor2icc, 7
peach, 8
pear, 9
pepper, 10
*Topic **risk assessment**
pesticides-package, 2
apple, 2, 3, 4, 6, 7
appleAll, 3, 4
cdfDist, 2, 5, 7
cor2icc, 2, 6, 7
peach, 2, 6, 7, 8
pear, 2, 6, 7, 9
pepper, 2, 6, 7, 10
pesticides (pesticides-package), 2
pesticides-package, 2
plot.cdfDist (cdfDist), 5
print.cdfDist (cdfDist), 5
summary.cdfDist (cdfDist), 5